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Description

Method For Determining The Color Perception In Multilayer Systems

The invention relates to a method for determining the color effect of dispersive materials such as materials or biological substances of a multilayer system, in particular a series of layers in teeth or dental materials.

An objective of determining the color perception is an adaptation or an adjustment of the color effect of new multilayer systems in existing multilayer systems, for example, as a step of quality assurance or when developing and assessing new materials and their combinations. This applies to multilayer systems in the field of cosmetic or aesthetic medical applications, e.g. for dentures, up to technical fields, e.g. for automobile finishes or plastics. The color effect of a material system is dependent on the layer thickness and the back dispersion(remission) of the light and can be determined pursuant to DIN 5033 according to the parity, tristimulus or spectral method for different color systems, e.g. CIELAB or CIELUV. For example, measuring instruments such as color spectrometers or colorimeters can be used as well as a visual sampling, e.g. by means of special color scales as described e.g. for the dental field in DE A 196 46 923, DE-A 101 21 553 or DE-A 100 23 840.

Due to the technical manufacturing process to be carried out in multilayer systems and the combination of individual layers, the color effect cannot be compared directly, but only determined and assessed afterward, i.e. after it has been finished, when it is no longer possible to correct the color.

Therefore, to obtain a desired color effect and determine or predict the respective color effect in varying layer thicknesses, time-consuming and expensive series of measurements and tests by the manufacturer are generally required, also according to the trial and error principle. To avoid this, attempts are being made to calculate the color effect with aid of simulations. This can be accomplished with sufficient accuracy for individual layers and less complex material systems that only have a molecular dispersion due to their relatively homogeneous inner structure.

A calculation of this type for predicting the color effect for different layer thicknesses has thus far been carried out with aid of a Kubelka-Munk equation as a one-dimensional model for solving the radiation transport equation, both in the field of dental science and in the technical field, such as in the paint industry, as basis of, for example, concentration-dependent computer color matching. The

absorption coefficient A_{KM} and dispersion coefficient S_{KM} are calculated therewith from transmission or remission properties measured on material samples. The remission spectra for various layer thicknesses can be predicted on the basis of A_{KM} and S_{KM}, for example, in front of a white or black background or in front of a background defined according to a color system. The color effect can be calculated from the remission spectra dependent on the color system used. For example, the calculation of the color effect according to CIELAB pursuant to the standard DIN 5033 can be ascertained by converting the remission values into X, Y, Z tristimulus values and subsequently into CIELAB values. This conversion of measured remission values into CIELAB values is also integrated in the software of color spectrometers, as used in the paint industry. By comparing the CIELAB values and calculating the difference in color ΔE_{ab} pursuant to DIN standard 6074, variations in color between samples of the studied materials can be ascertained.

However, with the Kubelka-Munk equation, the measurement geometries of the measuring apparatus used for the transmission or remission measurements cannot be taken into consideration and simplified assumptions that are detrimental to accuracy can be made. This results in systematic errors which can become apparent in visible differences in color between simulation result and reality. However, the greatest disadvantage of the Kubelka-Munk theory is that only processes of surface reflection can be taken into consideration. For example, this is shown in Fig. 1 on the light path of a photon 1 after reflection of the light on the surface of a material layer 2 of predetermined thickness.

With the Kubelka-Munk equation, the actually existing conditions can no longer be correctly reproduced in multilayer systems in which structural - not molecular – dispersion geometries are present. In this case, due to the layer structure and the structure peculiarities, a light propagation with internal multiple dispersion processes results in the material. The remission and with it the color effect result from a very complex interaction of the optical properties of the different contents and components of the layers due to the light propagation by scattering, absorption and refraction on the boundary layers. By way of example, Fig. 2 shows the light path of a photon 1 and an alternative light path 1' after multiple scatterings within several successive material layers 2, 3, 4 of different thickness and type. Therefore, when using the Kubelka-Munk equation for multilayer systems with structure scattering, essential reservations concerning the accuracy of the prediction of the remission and thus the color effect must be accepted which become noticeable as visually perceivable differences. Therefore, to improve the predictable accuracy of the remission and thus the color effect, the development of a method is required which can correctly and accurately take this structurally-dependent multiple dispersion into consideration.

The object of the present invention is to more accurately than previously be able to calculate and

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thus predict the color perception for multilayer systems of combinations of various dispersive materials or biological substances consisting of combined, different layers with various optical properties for varying layer thickness without having to repeatedly produce samples consisting of the combined layer thicknesses of interest and to have to measure the color effect, e.g. in conventional color spectrophotometers, in each case.

In particular, the color perception for multilayer systems in the dental field should be calculated or predicted, whereby series of layers in teeth, e.g. enamel and dentine, in any layer thickness desired and dental materials, e.g. composites and ceramics, are of special interest.

To solve the object, the invention essentially provides that the remission of the multilayer system is calculated by means of Monte Carlo simulations based on the respective intrinsic optical parameters of the different materials of the layer system comprising dispersion coefficient μ_s, anisotropy factor g and corrected absorption coefficient μ_{ak} and including refractive index n, thickness d of the respective layer and dispersion phase function of the individual materials in each case.

The intrinsic optical parameters can thereby be determined based on spectrometric measurements or taken from a data bank.

According to the invention, a method is proposed with which the visual perception of the color of multilayer systems or the results of their measurement detection, e.g. by color spectrometer, can be accurately determined or predicted adequately. Surprisingly, it was shown that, in the presence of structural dispersion geometries in multilayer systems with simulation calculations according to the principle of the Monte Carlo simulation as three-dimensional solution approach of the radiation transport equation and a subsequent special correction process, a more correct and essentially accurate determination of the color perception is possible than previously.

The optical properties of the respective materials or biological substances contained in the multilayer system serve as initial data in the form of intrinsic optical parameters absorption coefficient μ_a, dispersion coefficient μ_s and anisotropy factor g.

To determine the intrinsic optical parameters - also called microscopic parameters - which are independent of the material thickness, methods can be used which are known from tissue optics for dosimetric calculations in medicinal laser therapies. Thus, a calculation can be made with aid of an inverse Monte Carlo simulation from the macroscopic optical parameters, such as the diffuse remission R_d, the total transmission T_t, the diffuse transmission T_d or the collimated transmission T_c which were measured in an Ulbricht sphere-type spectrometer on samples having a previously

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ascertained suitable sample thickness d.

In particular, it is provided that the intrinsic optical parameters dispersion coefficient μ_s (uncorrected), absorption coefficient μ_a and anisotropy factor g of a material based on the macroscopic optical parameters of the material in the form of, in particular, diffuse remission R_d, diffuse transmission T_d and/or total transmission T_t and/or the collimated transmission T_c, taking the dispersion phase function of the material into consideration, thickness d of a layer of the material used for determining the macroscopic parameters and refractive index n of the material can be calculated by means of inverse Monte Carlo simulation.

After that, the dispersion phase function and the refractive index n of the material can be calculated by means of inverse Monte Carlo simulation of the corrected absorption coefficient μ_{ak} for each material on the basis of both intrinsic optical parameters dispersion coefficient μ_s and anisotropy factor go as well as the remission of an optically dense layer consisting of the material, having a thickness d_D and taking into consideration at least the thickness d_D. The dispersion coefficient μ_s and the anisotropy factor g are already known from the previously completed calculation.

In other words, according to the invention, the calculated absorption coefficient μ_a is corrected with aid of the remission values of an optically denser sample of the test thickness d_D of the material to be studied together with the determined values of μ_s and g in a renewed inverse Monte Carlo simulation for the corrected absorption coefficient μ_{ak}. The accuracy of the calculation of the color effect is substantially increased by this step.

The absorption can be calculated all the more accurately the greater the thickness of a layer. However, to determine the initial data μ_a, μ_s and g, no optically dense sample may be used for the spectrometric measurement since a certain percentage of collimated transmission, i.e. transparency, is required for this simulation process.

The data concerning the intrinsic optical parameters can be provided in a data bank in expansion of the basic idea of the invention in dependency on the material. When setting up a data bank of this type which contains the intrinsic optical parameters μ_{ak}, μ_s and g for different materials or biological substances or dental materials, reference can be made to these values, so that spectrometric measurements are no longer required when using these materials in a multilayer system for determining their color effect.

Subsequently, based on μ_{ak}, μ_s and g, the remission for a multilayer system can be calculated by a forward Monte Carlo simulation at an selectable wavelength and respectively selectable thicknesses

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of the layers contained in the multilayer system. Instead of the remission, the calculation of the transmission is also possible. The wavelength-dependent values of the remission can be transformed into color values e.g. the coordinates according to CIELAB or other color systems by means of suitable algorithms. It is also possible to use multifactor analysis to determine the color effect according to new, alternative color systems.

Moreover, it is possible to calculate the color effect for different and freely selectable measurement geometries.

The color effect can thus be determined with the described procedure with a much higher accuracy than previously for a multilayer system as a combination of various materials or biological substances of, in particular, dental or dentotechnical series of layers for varying layer thicknesses of the individual layers since, on the one hand, the multiple scatterings produced by the internal structure dispersion in the different layers can be correctly calculated and, on the other hand, the accuracy further increased by the determination of the corrected absorption coefficient μ_{ak}. In this way, it is possible to predict the color effect for multilayer systems so accurately that visual differences can no longer be perceived. As a result, with known material behaviour, the color effect of a multilayer system can already be precisely predicted for selectable layer thickness combinations prior to production of said multilayer system. Moreover, the measuring geometry can be taken into consideration and thus also the result of layer thickness-dependent measurements in different spectrometers, for example, of remission measurements in color spectrometers, can be predicted.

The method is especially suitable for use in multilayer systems in dentistry to determine the color of dental restoration materials and tooth color in which an especially high accuracy is required due to the very fine color gradations of e.g. reddish, yellowish or greyish white. Both teeth and dental prosthesis materials show a layer structure and complex inner dispersion geometries due to their structural composition. Teeth consist of the hard tooth substances enamel and dentine with prism or tubular structure. Dental prosthesis materials are also composed of layers of varying opacity to duplicate the resultant optical impression for an optimal aesthetic with a complex structure consisting of filling materials of the most varied types and forms which are embedded in a matrix.

The described method which is distinguished by the calculation of the remission for multilayer systems with successive different material layers of selectable layer thickness and properties takes place by means of Monte Carlo simulations based on the intrinsic optical parameters having a corrected absorption coefficient μ_{ak}, dispersion coefficient μ_s and anisotropy factor g as well as the refractive index n and including the dispersion phase function for considering the internal multiple material dispersion can also be used on all other multilayer systems with structural scatter, both in

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the biological and technical fields or in other systems. The color effect of e.g. layers which do not extend in a straight but in a curved plane can also be calculated or predicted thereby.

Further details, advantages and features of the invention can be found in the claims, the features found therein - alone and/or in combination - and also in the following description of the embodiments found in the drawings, showing:

Fig. 1   a schematic representation of a light path after surface reflection on a material layer,

Fig. 2   schematic representation of light paths in material layers,

Fig. 3   a basic representation of a test room with an Ulbricht sphere,

Fig. 4   a flow diagram for calculating intrinsic optical parameters,

Fig. 5   a flow diagram for inverse Monte Carlo simulation, and

Fig. 6   a flow diagram for calculating the remission and subsequently the color effect of a multilayer system.

According to the invention, to determine the color effect of dispersion layers of different materials on the basis of remission spectra, intrinsic (microscopic) optical parameters absorption coefficient μ_a, dispersion coefficient μ_s and anisotropy factor g of the materials, whether due to calculations on the basis of experimentally ascertained macroscopic optical parameters or taking values found in data banks into consideration, on the basis of which Monte Carlo simulations are carried out. The Monte Carlo simulation is a numerical method with high accuracy used for solving equation systems and statistical processes.

In this way, intrinsic optical parameters can be calculated on the basis of measured macroscopic optical parameters by means of an inverse Monte Carlo simulation with aid of e.g. a simulation software WinFit 32, Version 5.2. developed by Roggan. To measure the macroscopic optical parameters, an Ulbricht sphere-type spectrometer in the form of a double-beam spectrometer can be used, as found in principle in Fig. 3.

Thus, a test room 10 is shown in Fig. 3 in which an Ulbricht sphere 12 is arranged. Furthermore, reference beam 14 and test beam 16 are drawn in. The reference beam 14 is led via mirror S3', S4' and S5' into the Ulbricht sphere 12 to calibration to a reference standard 18. The Ulbricht sphere 12 and reference standard 18 can consist of spectralon, as a result of which a 99.8% reflection of the

light is possible for an almost loss-free detection of the photons.

Via Mirrors S1' and S2', the test beam 16 reaches a test piece (not shown) having a thickness d and into the Ulbricht sphere 12 after having passed through a selectable beam-focussing optical lens 20. The measured values are standardized by the successive emission of a test beam 16 and reference beam 14 automatically with each measured value. The name double-beam spectrometer results from this.

The test piece is fastened in the sample holder either at the transmission port 22 or at the remission port 24 of the Ulbricht sphere 12, dependent on whether or not forward or backward dispersion is to be measured. The respectively selected optical lens 20 regulates the focussing of the light spot on the transmission and remission port 22, 24.

The macroscopic optical parameters diffuse remission R_d, diffuse transmission T_d and total transmission T_t can then be measured with a corresponding arrangement. Alternatively, when using another correspondingly constructed Ulbricht sphere-type spectrometer - or an experimental structure with an Ulbricht sphere - in addition to R_d and T_t, the collimated transmission T_c can also be measured instead of the diffuse transmission T_d. The corresponding macroscopic optical parameters are defined as follows. When a ray of light hits, a distribution of the photons which is specific for the respective medium forms in the radiation volume. A part of the radiation is absorbed. A further part of the photons is scattered in the medium. The dispersion can be subdivided into back dispersion as diffuse remission R_d and forward dispersion as diffuse transmission T_d. With a thin layer thickness, photons are also transmitted without a prior dispersion as collimated transmission T_c. The sum of collimated and diffuse transmission produces the total transmission T_t ($T_d + T_c = T_t$). These macroscopic parameters are dependent on wavelength, material and layer thickness.

For materials which are used in layer systems, corresponding macroscopic optical parameters are determined. The intrinsic optical parameters of the material, i.e. absorption coefficient μ_a, dispersion coefficient μ_s and anisotropy factor g, are then determined by inverse Monte Carlo simulation from the macroscopic optical parameters diffuse remission R_d, diffuse transmission T_d and/or total transmission T_t and/or collimated transmission T_c - two of the transmission parameters must be known ($T_d + T_c = T_t$). In the inverse Monte Carlo simulation, dispersion phase function of the material, test thickness d of the material, refractive index n of the material and measurement geometry are thereby taken into consideration.

When using an Ulbricht sphere-type spectrometer, measurement geometry means e.g. sample

geometry, diaphragm diameter, sphere parameter, beam divergence and diameter of the light spot. In other words, existing geometric and optical conditions are taken into consideration in the simulation during measuring, so that systematic errors are avoided and the accuracy of the simulation is increased. In particular, by taking measurement geometry into consideration, e.g. lateral losses of photons on the surface area of the test piece can also be included.

A clear determination of the intrinsic optical parameters requires the measuring of three independent values such as R_d, T_t and T_c or T_d.

The Heney-Greenstein phase function or the Reynolds-McCormick phase function can be used as dispersion phase function. Other suitable dispersion phase functions, which are typical for the respective material, may also be considered.

In addition to a mathematical formula, the dispersion phase function may also consist of a "look up table", i.e. determination of the dispersion probability via the angle between the direction of the photon to the dispersion occurrence and the direction after the scattering. As a result, a suitable dispersion phase function can be determined for each material. A dispersion phase function may by all means be suitable for several materials, i.e. not be definitely restricted to one material. For example, the Heney-Greenstein function is usually used for a number of biological tissues. However, when g is especially high, it may be advantageous to use the Reynolds-McCormick function.

The inverse Monte Carlo simulation can again be found in Fig. 5. In principle, the inverse Monte Carlo simulation works in such a way that one proceeds from intrinsic optical parameter values which are then calculated back to the measured or available macroscopic optical parameters. If a difference results that is smaller than an error limit, then the basic intrinsic optical parameters are accepted.

The intrinsic optical parameters can be determined accordingly to suitable materials.

If, for example, the remission and thus the color effect of a system according to Fig. 2, comprising three different material layers 2, 3, 4, is to be determined, i.e. predicted, the intrinsic optical parameter of each material is then taken as a basis for a forward Monte Carlo simulation. Furthermore, during this simulation, the measurement geometries both for each material the dispersion phase function of each material and the refractive index n of the materials are taken into consideration. Furthermore, the thicknesses d_1, d_2, d_3 of the layers 2, 3, 4 are entered. The thickness of each layer per se is thereby constant.

A wavelength-dependent remission then results from the forward Monte Carlo simulation, the color effect, i.e. the color values according to a selected color system such as CIELAB, are then calculated from said remission by appropriate calculation algorithms or multifactor analysis.

To obtain greater accuracy, it is provided according to the invention that the absorption coefficient be corrected; since with the measurements performed according to Fig. 3, the test pieces must have a thickness that enables a transmission of light. However, the absorption can be determined all the more accurately the greater the thickness of a layer. Therefore, the dispersion coefficient μ_s and the anisotropy factor g, which were calculated by means of inverse Monte Carlo simulation according to Figs. 4 and 5, as well as the remission of an optically dense test piece having a thickness d_D are subjected to a further inverse Monte Carlo simulation on the basis of which a corrected absorption coefficient μ_{ak} is now determined. During simulation, dispersion phase functions of the material, sample thickness d_D, refractive index n of the material and the measurement geometry are also taken into consideration. This can be seen in the upper part of Fig. 6.

Consequently, for a multilayer system, the calculation shown in principle in the area 26 of the flow diagram of Fig. 6 is performed according to the number of layers or different materials in order to then calculate the remission of the layer system by forward Monte Carlo simulation according to previous explanations on the basis of corresponding material-specific intrinsic optical parameters, i.e. corrected absorption coefficient μ_{ak}, dispersion coefficient μ_s and anisotropy factor g of the materials, whereby the dispersion phase function, refractive index n_x as well as layer thicknesses d_x and number x of layers of the various materials are taken into consideration, optionally also the measurement geometry.

In this way, the remission of the entire system of all layers is calculated in their geometric sequence, so that, as noted, the phase functions and refractive indices of the materials of the layers having the desired thicknesses and number of layers are to be taken into consideration. The color effect then results from the remission according to e.g. DIN 5033 Farbmessung, Part 1 - 9, Beuth Verlag Berlin, 1979 - 1992.

List of References

1	Light path
1'	Alternative light path
2	First material layer
3	Second material layer
4	Third material layer
10	Test room
12	Ulbricht sphere
14	Reference beam
16	Test beam
15', 52', 53', 54', 55' Mirror	
18	Reference standard
20	Lens
22	Transmission port
24	Remission port
26	Area of Fig. 6
ΔE_{ab}	Difference in color according to CIELAB
μ_a	Absorption coefficient
μ_{ak}	Corrected absorption coefficient
μ_s	Dispersion coefficient
A_{KM}	Kubelka-Munk absorption coefficient
d, d_1, d_2, d_3	Thickness of test piece
d_D	Thickness of test piece of an optically dense sample
g	Anisotropy factor
n	Refractive index
R_d	Diffuse remission
S_{KM}	Kubelka-Munk dispersion coefficient
T_c	Collimated transmission
T_d	Diffuse transmission
T_t	Total transmission